Magnetic behavior of a spin-1 Blume-Emery-Griffiths model

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Abstract. I study the one-dimensional spin-1 Blume-Emery-Griffiths model with bilinear and biquadratic exchange interactions and single-ion crystal field under an applied magnetic field. This model can be exactly mapped into a tight-binding Hubbard model - extended to include intersite interactions - provided one renormalizes the chemical and the on-site potentials, which become temperature dependent. After this transformation, I provide the exact solution of the Blume-Emery-Griffiths model in one dimension by means of the Green's functions and equations of motion formalism. I investigate the magnetic variations of physical quantities - such as magnetization, quadrupolar moment, susceptibility - for different values of the interaction parameters and of the applied field, focusing on the role played by the biquadratic interaction in the breakdown of the magnetization plateaus.

1. Introduction

The Blume-Emery-Griffiths (BEG) model is a spin-1 model which presents a rich variety of critical and multicritical phenomena [1]. This model has been used to describe systems characterized by three states per spin, and it was originally introduced to describe the phase separation and superfluidity in the ^{3}He-^{4}He mixtures. The BEG model can also describe the properties of a variety of systems ranging from spin-1 magnets to liquid crystal mixtures, semiconductor alloys, microemulsions, to quote a few. The spin-1 BEG model is characterized by a bilinear (J) and biquadratic (K) nearest-neighbor pair interactions and a single-ion potential (Δ). The one-dimensional case for the BEG model was studied in Ref. [2], where exact renormalization-group recursion relations were derived, exhibiting tricritical and critical fixed points.

The underlying idea of this paper is to provide a new and general framework to exactly investigate the one-dimensional BEG model in the whole parameters space. For one-dimensional lattices, or more generally for lattices with no closed loops, classical fermionic and spin systems can be easily solved by means of the transfer matrix method [3]. As it is well known, the partition function of a 1d model of a classical spin-1 system with nearest-neighbor interactions can be calculated from the largest eigenvalue of a 3×3 matrix. However, this method is hardy implementable when more complex lattices are considered. The Onsager solution for the two-dimensional Ising model is an emblematic example [4]. Thus, there is the necessity to foster alternative methods which can be used for a large class of lattices. Recently, it has been shown that, upon transforming to fermionic variables, spin systems can be conveniently studied by

means of quantum field methods, namely: Green's functions and equations of motion methods [5]. This approach has the advantage of offering a general formulation for any dimension and to provide a rigorous determination of a complete set of eigenoperators of the Hamiltonian and, correspondingly, of the set of elementary excitations.

The aim of the present paper is twofold. First, I would like to further develop our previous work [6], where the finite temperature phase diagrams of the one-dimensional BEG model with vanishing biquadratic exchange have been obtained, by extending it to a more general situation with a finite biquadratic interaction. Secondly, the BEG model exhibits interesting features when one considers a non-zero biquadratic coupling, such as the breakdown of magnetic plateaus. Here, I address the problem of determining the effect on the behavior of thermodynamic quantities of the presence of a finite biquadratic interaction. I study the properties of the system as functions of the external parameters J, T, Δ and h allowing for the biquadratic interaction K to be both repulsive and attractive.

2. The model

The BEG model consists of a system with three states per spin. For nearest-neighbor interaction, the one-dimensional BEG model is described by the Hamiltonian

$$H = -J\sum_{\mathbf{i}} S(i)S(i+1) - K\sum_{\mathbf{i}} S^2(i)S^2(i+1) + \Delta\sum_{\mathbf{i}} S^2(i) - h\sum_{\mathbf{i}} S(i), \qquad (1)$$

where the spin variable $S(i)$ takes the values $S(i) = -1, 0, 1$. I use the Heisenberg picture: $i = (\mathbf{i}, t)$, where $\mathbf{i}$ stands for the lattice vector $\mathbf{R_i}$. This model can be mapped, in two steps, into a fermionic model: namely, the Hubbard model (in the limit of zero bandwidth) with local interaction U and extended to include intersite, charge-charge, charge-double occupancy and double occupancy-double occupancy interactions [6]. Firstly, by means of the transformation $S(i) = [n(i) - 1]$, where $n(i) = \sum_\sigma c_\sigma^\dagger(i)c_\sigma(i) = c^\dagger(i)c(i)$ is the density number operator of a fermionic system. $c(i)$ $(c^\dagger(i))$ is the annihilation (creation) operator of fermionic field in the spinor notation and satisfies canonical anti-commutation relations. Secondly, by taking into account the four possible values of the particle density $(n(i) = 0$, $n_\uparrow(i) = 1$ and $n_\downarrow(i) = 1$, $n(i) = 2)$, one redefines the chemical potential as $\mu = \mu' - \beta^{-1}\ln 2$ and the on-site potential as $U = U' - 2\beta^{-1}\ln 2$, where $\beta = 1/k_B T$. I refer the interested reader to Ref. [6, 7] for a detailed analysis of the mapping between the extended Hubbard model and spin-1 Ising model. Once the BEG model has been mapped into the fermionic model, the latter can be exactly solved by means of the Green's function and equations of motion formalism. Upon introducing the Hubbard projection operators $\xi(i) = [1 - n(i)]c(i)$, and $\eta(i) = n(i)c(i)$, one can define composite multiplet operators $\psi^{(\xi)}(i)$ and $\psi^{(\eta)}(i)$ which are eigenoperators of the fermionic Hamiltonian with eigenenergies $\varepsilon^{(\xi)}$ and $\varepsilon^{(\eta)}$ [6]. As a consequence, an exact solution of the Hamiltonian can be formally obtained. Within this framework, the retarded Green's function and pertinent correlation functions turn out to be functions of only two parameters, in terms of which one may find a solution of the model. I refer the interested reader to Ref. [6] for computational details.

3. Magnetic Responses

By exploiting the general formulation sketched in the previous section, I shall now study the magnetic properties of the 1D BEG model, by restricting the analysis to the case $J < 0$. In the following, I set $J = -1$ and I consider only positive values of h, owing to the symmetry property of the model under the transformation $h \rightarrow -h$ and $S \rightarrow -S$. When $K = 0$ and $\Delta = 0$, the ground state is purely antiferromagnetic for $0 \leq h < 2|J|$. By varying the magnetic field, the system undergoes a phase transition to a paramagnetic state at $h = \pm 2|J|$. As a consequence, the magnetization, defined as

$$m = \langle S(i) \rangle = \langle n(i) \rangle - 1, \qquad (2)$$
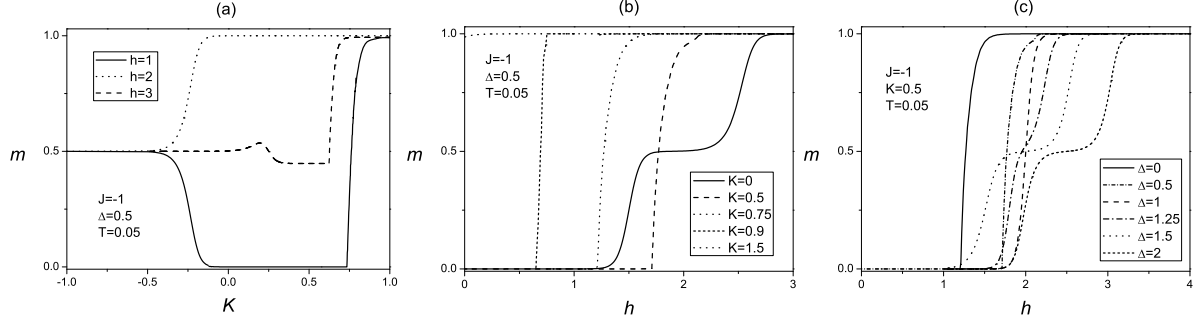
Figure 1. (a) The magnetization m as a function of the biquadratic interaction K for $J = -1$, $T = 0.05$, $\Delta = 0.5$, and $h = 1, 2, 3$. (b) The magnetization as a function of the external field h for $J = -1$, $T = 0.05$, $\Delta = 0.5$ and positive values of K. (c) The magnetization as a function of the external field for $J = -1$, $T = 0.05$, $K = 0.5$ and several values of Δ.

presents, at $T = 0$, two plateaus as a function of the external field h. When the anisotropy Δ is turned on (keeping $K = 0$), one observes three plateaus at $m = 0$, $m = 1/2$ and $m = 1$ [6, 8]. The intermediate phase between the antiferromagnetic and paramagnetic ones has a width depending on Δ, whose endpoints are denoted by h_c and h_s, i.e., starting point of a nonzero magnetization and saturated field, respectively. For finite biquadratic interaction, the presence of plateaus in the magnetization curve dramatically depends on the sign of the interaction itself and on the value of the anisotropy.

In Fig. 1a, I plot the magnetization as a function of the biquadratic exchange at $\Delta = 0.5$ for values of the magnetic field belonging to the three different plateaus observed at $K = 0$. For all values of h, one observes that, for large positive biquadratic coupling, all the spins are aligned along the magnetic field ($m = 1$). On the other hand, for large negative biquadratic coupling, half of the spins are parallel to h and the other half lies in the transverse plane. In the intermediate region, according to the strength of the biquadratic coupling, one observes one, two or three plateaus. The range of this intermediate region depends on Δ, and for $\Delta \geq 1$ only one plateau at $m = 1/2$ is observed for $K < 0$. In Fig. 1b, I plot the magnetization as a function of the magnetic field at $T = 0.05$, $\Delta = 0.5$ for different values of K. Starting from $K = 0$, by turning on a finite biquadratic exchange, one observes that the width of the intermediate plateau shrinks and vanishes ($h_c = h_s$). Further augmenting K, one observes the decrease of h_s, which eventually vanishes for sufficiently large K: the spins are all polarized in the h direction as soon as the magnetic field is turned on. However, the three plateau scenario can be restored by varying the anisotropy, as it is evident from Fig. 1c, where I plot the magnetization as a function of the magnetic field at low temperature for $K = 0.5$. For fixed Δ, the width of the $m = 1/2$ plateau decreases by increasing K. On the other hand, for fixed K, the width of the intermediate plateau augments by increasing Δ in the range $0 < \Delta < 1$ and becomes independent of Δ for $\Delta > 1$. For these ranges of the parameters, the critical field h_c and the saturated field h_s satisfy the laws: $h_c = 2 - \Delta$, $h_s = 2 + \Delta$. To further analyze the magnetic behavior of the system, I have studied the quadrupolar moment Q, defined as

$$Q = \langle S^2(i) \rangle. \tag{3}$$

In the limit $T \to 0$, and for $K = 0$, also this quantity shows plateaus for $\Delta \geq 0$. In Fig. 2a the quadrupolar moment Q is plotted as a function of the external magnetic field, for $\Delta = 0.5$, $J = -1$, $T = 0.05$ and for various values of K. At $K = 0$, Q takes the value $1/2$ in the range $h_c < h < h_s$, whereas is equal to 1 for all other values of h. Upon increasing the value of the
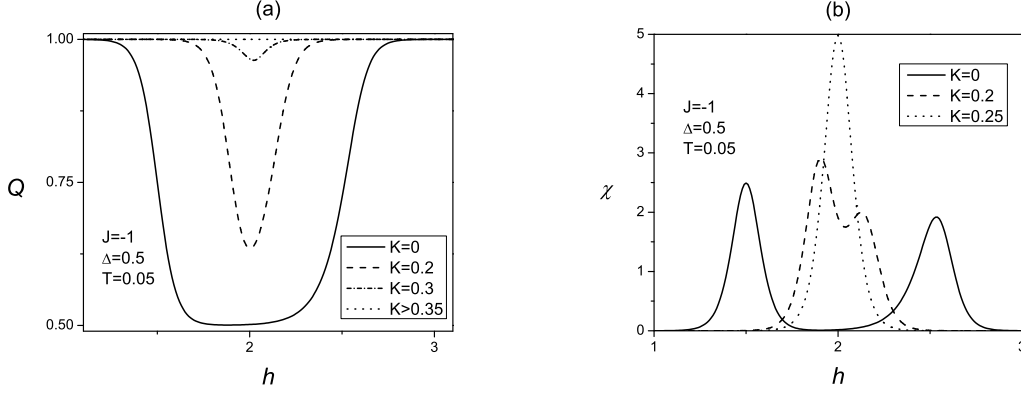
Figure 2. (a) The quadrupolar moment Q as a function of the magnetic field for $J = -1$, $\Delta = 0.5$, $T = 0.05$ and positive values of the biquadratic interaction. (b) The magnetic susceptibility χ as a function of the magnetic field for $J = -1$, $\Delta = 0.5$, $T = 0.05$ and positive values of the biquadratic interaction.

biquadratic coupling, one observes the breakdown of the intermediate plateau, resulting in a uniform quadrupolar moment for all values of the magnetic field. For strong anisotropy, the quadrupolar moment shows the same S-shape curve characterizing the magnetization and one finds $Q = m$. The possible breakdown of the magnetic plateaus can also be evidenced by looking at the peak(s) found in the magnetic susceptibility $\chi = dm/dh$. As evidenced in Fig.2b, when plotted as a function of the magnetic field, χ shows two peaks at low temperature at h_c and h_s - for $K = 0$ and $\Delta = 0.5$ - signalling a step-like behavior of the magnetization. By increasing K one observes that the two peaks merge into only one peak: the intermediate plateau at $m = 1/2$ has disappeared.

4. Concluding Remarks

I have evidenced how the use of the Green's function and equations of motion formalism leads to the exact solution of the one-dimensional BEG model. The analysis allows for a comprehensive study of the model in the whole space of parameters K, J, Δ, h and T. Here, I have focused on the antiferromagnetic properties exhibited by the model and I have shown that the three zero-temperature magnetic plateaus scenario exhibited by the model when $\Delta > 0$ and $K = 0$ may break down for sufficiently large positive and negative biquadratic interaction K. However, a large anisotropy can restore the three plateaus scenario also for finite K. This scenario is endorsed by the behavior of the quadrupolar moment Q and of the susceptibility χ.

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